Integrated Polyharmonic Spline RBF Simulation of High-Dimensional PDE for Phonon Transport

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Abstract

In the past, qmultiquadrics (MQ) is considered one of the most effective radial basis functions (RBFs). However, the accuracy of the numerical approximation using the MQ or any other RBFs containing the shape parameters is highly affected by the choice of the shape parameters. One of the alternatives to avoid dealing with the shape parameters is to use the polyharmonic spline RBF that contains no shape parameter in the approximation process. Using this approach, the problem of determination of the shape parameters naturally disappeared.

The integrated polyharmonic splines will be applied to the Boltzmann Transport Equation (BTE) of phonons in 6D real and momentum space for thermal simulation of a semiconductor nano-structure. Phonons are quantum representations of crystal lattice vibrations excited by thermal energy. The phonon density distribution thus represents the temperature distribution in a domain structure. The BTE has been a challenging problem in many engineering fields involving particle transport for electrons, ionized molecules, phonons, etc.

The meshless approach on the other hand is a newly developed research area in computational partial differential equations (PDEs) starting in the 1990's. It has recently attracted significant attention in many fields such as fluid dynamics, solid mechanics, and computational mathematics due to its flexibility for complicated problems in high-dimensional space. Our preliminary results show that the proposed RBF basis of the solution space is very effective and accurate for high-dimensional PDEs for Phonons.

Keywords: Radial Basis Function, Polyharmonic Spline, Boltzmann Transport Equation, Phonon Transport, Temperature Distribution in Nanostructures.